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     (FILE 'HOME' ENTERED AT 12:23:38 ON 03 FEB 2005)

     FILE 'HCAPLUS' ENTERED AT 12:24:05 ON 03 FEB 2005
                E BHANDARI K/AU
L1           58 E3-8
                E SRIVASTAVA S/AU
L2         2243 E3-22
                E SRIVASTAVA SHIPRA/AU
L3            1 E3
                E NATH C/AU
L4           67 E3-4
L5         8868 (COUNC? (1A) SCI? (1A) IND? (1A) RES?)/CS,PA
L6           32 L1-4 AND ?UREA/BI
L7            0 L6 AND ?ARYLOXY?/BI
L8           11 L6 AND PREP+NT/RL

     FILE 'WPIX' ENTERED AT 12:29:11 ON 03 FEB 2005
                E BHANDARI K/AU
                E SRIVASTAVA S/AU
L9           91 E3-10
                E NATH C/AU
L10           4 E3
L11        1163 (COUNC? (1A) SCI? (1A) IND? (1A) RES?)/CS,PA
L12       25583 (B10-A13? OR C10-A13? OR E10-A13?)/MC OR (C07C273 OR C07C275)/I
L13           9 L9-11 AND L12

     FILE 'REGISTRY' ENTERED AT 12:37:10 ON 03 FEB 2005

     FILE 'HCAPLUS' ENTERED AT 12:37:15 ON 03 FEB 2005
L14             TRA L8 1- RN :      245 TERMS

     FILE 'REGISTRY' ENTERED AT 12:37:16 ON 03 FEB 2005
L15          245 SEA L14

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FILE LAST UPDATED: 2 Feb 2005  (20050202/ED)

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substance identification.

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L8 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:561475 HCAPLUS
DN 141:218306
ED Entered STN: 14 Jul 2004
TI Synthesis of tetrahydronaphthyl thioureas as potent appetite suppressants
AU **Bhandari, Kalpana**; **Srivastava, Shipra**; Shankar, Girija
CS Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow, 226001, India
SO Bioorganic & Medicinal Chemistry (2004), 12(15), 4189-4196
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Ltd.
DT Journal
LA English
CC 1-3 (Pharmacology)
AB A series of **thiourea** derivs. (7-23, 25-27) of 1-aminotetrahydronaphthalene (4) and 1-amino-2-hydroxytetrahydronaphthalene (5) were synthesized in single pot in 48-90% yield and evaluated for their anorexigenic activity. Among them compds. 10, 14, 15, 16 and 22 exhibited significant anorexigenic activity without any antidepressant effect and provided a new structural lead for appetite suppressants.
ST synthesis structure activity anorexic tetrahydronaphthyl **thiourea**
IT Appetite depressants
Structure-activity relationship
(synthesis of tetrahydronaphthyl thioureas as potent appetite suppressants)
IT 16112-96-2 61451-94-3 141034-13-1 745072-14-4
RL: PAC (Pharmacological activity); BIOL (Biological study)
(synthesis of tetrahydronaphthyl thioureas as potent appetite suppressants)
IT 2217-40-5 13286-65-2
RL: PAC (Pharmacological activity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(synthesis of tetrahydronaphthyl thioureas as potent appetite suppressants)
IT 58490-71-4P 141034-11-9P
RL: PAC (Pharmacological activity); RCT (Reactant); **SPN (Synthetic preparation)**; BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or reagent)
(synthesis of tetrahydronaphthyl thioureas as potent appetite suppressants)
IT 91215-19-9P 377765-08-7P 452969-06-1P 745072-15-5P 745072-16-6P 745072-17-7P 745072-18-8P 745072-19-9P 745072-20-2P 745072-21-3P 745072-22-4P 745072-23-5P 745072-24-6P 745072-25-7P 745072-26-8P 745072-27-9P 745072-28-0P 745810-28-0P
RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**; BIOL (Biological study); **PREP (Preparation)**
(synthesis of tetrahydronaphthyl thioureas as potent appetite suppressants)
IT 62-53-3, Aniline, reactions 64-04-0, 2-Phenylethylamine 92-54-6, Phenylpiperazine 103-67-3, Benzylmethylamine 108-91-8, Cyclohexylamine, reactions 109-07-9, 2-Methylpiperazine 123-75-1,

Pyrrolidine, reactions 2252-63-3, 1-[(4-Fluoro)phenyl]piperazine 6321-23-9, 4-Methylcyclohexylamine 6640-24-0, 1-[(3-Chloro)phenyl]piperazine 15532-75-9 34803-66-2, 1-(2-Pyridyl)piperazine 39593-08-3, 1-[(4-Methyl)phenyl]piperazine
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of tetrahydronaphthyl thioureas as potent appetite suppressants)

IT 745072-29-1P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(synthesis of tetrahydronaphthyl thioureas as potent appetite suppressants)

IT 7480-36-6P 745072-30-4P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(synthesis of tetrahydronaphthyl thioureas as potent appetite suppressants)

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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L8 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:160091 HCAPLUS
DN 139:69333
ED Entered STN: 04 Mar 2003
TI Molecular adducts of some triphenyltin(IV) O,O'-alkylene dithiophosphates
AU **Srivastava, S. K.**; Pandey, Y.
CS Sch. of Stud. in Chem., Jiwaji Univ., Gwalior, 474 011, India
SO Journal of the Indian Chemical Society (2003), 80(1), 38-39
CODEN: JICSAH; ISSN: 0019-4522
PB Indian Chemical Society
DT Journal
LA English
CC 29-8 (Organometallic and Organometalloidal Compounds)
OS CASREACT 139:69333

AB The interactions of triphenyltin(IV) O,O'-alkylenedithiophosphates, [(C6H5)3SnS(S)POQO], (Q = -CH2CHMe-, -CH2(CH2)3CH2- and -CMe2CMe2-) with various N, O and S donor Lewis bases have yielded new stable mol. adducts. The results suggest five- and six-coordinated Sn atom in case of unidentate and bidentate Lewis bases, resp.

ST triphenyltin alkylenedithiophosphate addn nitrogen oxygen sulfur donor Lewis base

IT Phosphates, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(O,O'-alkylenedithiophosphates; interactions of triphenyltin(IV) alkylene dithiophosphates with various N, O and S donor Lewis bases gave stable mol. adducts containing five- and six-coordinated Sn atoms)

IT Addition reaction
(interactions of triphenyltin(IV) alkylene dithiophosphates with various N, O and S donor Lewis bases gave stable mol. adducts containing five- and six-coordinated Sn atoms)

IT Lewis bases
RL: RCT (Reactant); RACT (Reactant or reagent)
(interactions of triphenyltin(IV) alkylene dithiophosphates with various N, O and S donor Lewis bases gave stable mol. adducts containing five- and six-coordinated Sn atoms)

IT Coordination number
(six; interactions of triphenyltin(IV) alkylene dithiophosphates with various N, O and S donor Lewis bases gave stable mol. adducts containing five- and six-coordinated Sn atoms)

IT 60-80-0, Antipyrine 62-56-6, **Thiourea**, reactions 66-71-7, 1,10-Phenanthroline 67-68-5, Dimethyl sulfoxide, reactions 68-12-2, Dimethylformamide, reactions 127-19-5, Dimethylacetamide 137-26-8, Tetramethylthiuramdisulfide 366-18-7, 2,2'-Bipyridyl 791-28-6, Triphenylphosphine oxide 872-50-4, reactions 1073-23-0, 2,6-Lutidine-N-oxide 3878-45-3, Triphenylphosphine sulfide 89202-03-9 356043-44-2 356043-45-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(interactions of triphenyltin(IV) alkylene dithiophosphates with various N, O and S donor Lewis bases gave stable mol. adducts containing five- and six-coordinated Sn atoms)

IT 551951-24-7P 551951-25-8P 551951-26-9P 551951-27-0P 551951-28-1P
551951-29-2P 551951-30-5P 551951-31-6P 551951-32-7P 551951-33-8P
551951-34-9P 551951-35-0P 551951-36-1P 551951-37-2P 551951-38-3P
551951-39-4P 551951-40-7P 551951-41-8P 551951-42-9P 551951-43-0P
551951-44-1P 551951-45-2P 551951-46-3P 551951-47-4P 551951-48-5P
551951-49-6P 551951-50-9P 551951-51-0P 551951-52-1P 551951-53-2P
551951-54-3P 551951-55-4P 551951-56-5P 551951-57-6P 551951-58-7P
551951-59-8P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(interactions of triphenyltin(IV) alkylene dithiophosphates with various N, O and S donor Lewis bases gave stable mol. adducts containing five- and six-coordinated Sn atoms)

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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L8 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:603494 HCAPLUS
DN 138:306285
ED Entered STN: 13 Aug 2002
TI Study of the temperature and enthalpy of wax crystallization from middle distillate by DSC
AU **Srivastava, S. P.**; Butz, T.; Verma, P. S.; Purohit, R. C.; Rahimian, I.
CS Indian Institute of Petroleum, Dehra Dun, 248 005, India
SO Petroleum Science and Technology (2002), 20(7 & 8), 831-839
CODEN: PSTEFV; ISSN: 1091-6466
PB Marcel Dekker, Inc.
DT Journal
LA English
CC 51-3 (Fossil Fuels, Derivatives, and Related Products)
AB The temperature and enthalpy of the wax crystallization and of melting were studied in the middle distillate (boiling range: 250-375.degree.) obtained from the indigenous Bombay-High (Off-Shore) crude oil by using a differential scanning calorimeter (DSC). To have better understanding of the gel formation processes the broad distillate fraction was fractionated into five narrow fractions of 25.degree. interval each. From these narrow subfractions the sats. were separated from aroms. by column chromatog., and from sats. the n-paraffins were separated from iso- and cyclo-paraffins by **urea** adduction, to obtain the n-paraffins concs. (**urea** adductables)-the wax- and the saturated solvent portion-the UNA. The thermal behavior of narrow subfractions along with their **urea** adductables and. The solvent portions were studied and the wax appearance temperature (WAT) thus measured was compared with those obtained by optical microscopy and with the ASTM cloud point, wherever possible. To obtain a clearer picture of the solidification process, further study was done by preparing synthetic blends of **urea** adductables in different concns. in the resp. aromatic and iso- and cyclo-paraffinic solvents (UNA) and studying the thermal behavior of each blend. The variation in WAT with wax concentration as measured by DSC is identical with that measured by optical microscopy and the ASTM cloud point. However, DSC values are lower than microscopic values and higher than ASTM cloud point. The enthalpy of the blends with the same amount of wax in the aromatic and iso- and cyclo-paraffinic solvents indicated that it is higher in the saturated solvent in comparison to aromatic solvent. This confirms the fact that in an aromatic solvent the solubility of the wax is greater, and hence a comparatively lower WAT. The results are further discussed.
ST temp enthalpy wax crystn middle distillate DSC pour point; cloud point crystn paraffin middle distillate alkane fraction
IT Alkanes, preparation
RL: OCU (Occurrence, unclassified); PEP (Physical, engineering or chemical process); **PUR (Purification or recovery)**; PYP (Physical process); OCCU (Occurrence); **PREP (Preparation)**; PROC (Process)
(C10-C26; temperature and enthalpy of wax crystallization from middle distillate fractions by DSC)
IT Petroleum products
(fractions; temperature and enthalpy of wax crystallization from middle distillate fractions by DSC)
IT Petroleum products
(middle distillates, b.p. 250.degree. - 375.degree. cut; temperature and enthalpy of wax crystallization from middle distillate fractions by DSC)

IT Cloud point
Crystallization
Crystallization enthalpy
Crystallization temperature
Gelation
Melting point
Pour point
Solidification point
(temperature and enthalpy of wax crystallization from middle distillate fractions by DSC)
IT Aromatic hydrocarbons, preparation
RL: OCU (Occurrence, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); **PUR (Purification or recovery)**; PYP (Physical process); OCCU (Occurrence); **PREP (Preparation)**; PROC (Process)
(temperature and enthalpy of wax crystallization from middle distillate fractions by DSC)
IT Paraffin waxes, processes
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(temperature and enthalpy of wax crystallization from middle distillate fractions by DSC)
IT Hydrocarbons, preparation
RL: PEP (Physical, engineering or chemical process); **PUR (Purification or recovery)**; PYP (Physical process); **PREP (Preparation)**; PROC (Process)
(temperature and enthalpy of wax crystallization from middle distillate fractions by DSC)
IT Cycloalkanes
Isoalkanes
RL: OCU (Occurrence, unclassified); **PUR (Purification or recovery)**; RCT (Reactant); REM (Removal or disposal); OCCU (Occurrence); **PREP (Preparation)**; PROC (Process); RACT (Reactant or reagent)
(**urea** adduction; temperature and enthalpy of wax crystallization from middle distillate fractions by DSC)
IT 57-13-6, **Urea**, processes
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PROC (Process)
(temperature and enthalpy of wax crystallization from middle distillate fractions by DSC)
RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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L8 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:712305 HCAPLUS
DN 136:37696
ED Entered STN: 28 Sep 2001

TI Reactivity of phenylmercury-O,O'-alkylenedithiophosphate
AU **Srivastava**, S. K.; Saxena, S. B.; Jain, S.
CS School of Studies in Chemistry, Jiwaji University, Gwalior, 474 011, India
SO Journal of the Indian Chemical Society (2001), 78(7), 362-363
CODEN: JICSAH; ISSN: 0019-4522
PB Indian Chemical Society
DT Journal
LA English
CC 29-9 (Organometallic and Organometalloidal Compounds)
OS CASREACT 136:37696
AB The reactions of phenylmercury O,O'-alkylenedithiophosphate [cyclic] [C6H5HgS(S)POCH2(CH2)3CH2O] with various O- and S- donor Lewis bases L (L = DMSO, DMF, 2,6-lutidine N-oxide, 1-methyl-2-pyrrolidinone, triphenylphosphine oxide, dimethylacetamide, antipyrine, **thiourea**, triphenylphosphine sulfide, tetramethylthiuram disulfide) have yielded some new 1:1 [C6H5HgS(S)POCH2(CH2)3CH2O].cntdot.L mol. adducts. According to anal. and spectral studies, the L is coordinated to the Hg atom, which is 3-coordinate.
ST alkylenedithiophosphate phenylmercury Lewis base adduct prepn
IT Lewis bases
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of phenylmercury alkylenedithiophosphate with Lewis bases)
IT 60-80-0 62-56-6, **Thiourea**, reactions 127-19-5 137-26-8
791-28-6 872-50-4, reactions 1073-23-0 3878-45-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(coordination reaction with alkylenedithiophosphate with Lewis bases)
IT 215809-52-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(coordination reaction with oxygen and sulfur donor ligands)
IT 380496-14-0P 380496-15-1P 380496-16-2P 380496-17-3P 380496-18-4P
380496-19-5P 380496-20-8P 380496-21-9P 380496-22-0P 380496-23-1P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(reactions of phenylmercury alkylenedithiophosphate with Lewis bases)
RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Basin, C; Inorg Chim Acta 1983, V77, PL131
(2) Basin, C; Inorg Chim Acta 1987, V128, P69
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L8 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:302854 HCAPLUS
DN 135:61407
ED Entered STN: 29 Apr 2001
TI Molecular adducts of some phenylmercury(II)O,O'-alkylene dithiophosphates
AU **Srivastava**, S. K.; Saxena, S. B.; Jain, S.

CS School of Studies in Chemistry, Jiwaji University, Gwalior, 474 011, India
SO Indian Journal of Chemistry, Section A: Inorganic, Bio-inorganic, Physical, Theoretical & Analytical Chemistry (2001), 40A(4), 380-382
CODEN: ICACEC; ISSN: 0376-4710
PB National Institute of Science Communication, CSIR
DT Journal
LA English
CC 29-9 (Organometallic and Organometalloidal Compounds)
AB The interactions of phenylmercury O,O'-alkylene dithiophosphates, [C6H5HgS(S)POGO] (G = -CH2C(H)-CH3 and C(CH3)2(CH3)2C-) with various O- and S- donor Lewis bases (e.g., DMSO, DMF, 2,6-lutidine N-oxide, 1-methyl-2-pyrrolidinone, triphenylphosphine oxide, dimethylacetamide, antipyrine, **thiourea**, triphenylphosphine sulfide and tetra-Me thiuramdisulfide) yielded new mol. adducts. The elemental analyses and spectral (IR and 1H NMR) data suggest the presence of three - coordinated mercury atom.
ST phenylmercury alkylene dithiophosphate Lewis base adduct prepn
IT Lewis bases
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(complexes, mercury; preparation of phenylmercury alkylene dithiophosphate Lewis base adducts)
IT Lewis bases
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phenylmercury alkylene dithiophosphate Lewis base adducts)
IT Coordination number
(three; in phenylmercury alkylene dithiophosphate Lewis base adducts)
IT 60-80-0, Antipyrine 62-56-6, **Thiourea**, reactions 67-68-5, Dimethyl sulfoxide, reactions 68-12-2, Dimethylformamide, reactions 127-19-5, Dimethylacetamide 137-26-8, Tetramethyl thiuramdisulphide 791-28-6, Triphenylphosphine oxide 872-50-4, 1-Methyl-2-pyrrolidinone, reactions 1073-23-0, 2,6-Lutidine N-oxide 3878-45-3, Triphenyl phosphine sulfide 154923-00-9 215809-51-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(mol. adduct formation between phenylmercury alkylene dithiophosphates and Lewis bases)
IT 345653-95-4P 345653-96-5P 345653-97-6P 345653-98-7P 345653-99-8P
345654-00-4P 345654-01-5P 345654-02-6P 345654-03-7P 345654-04-8P
345654-05-9P 345654-06-0P 345654-07-1P 345654-08-2P 345654-09-3P
345654-10-6P 345654-11-7P 345654-12-8P 345654-13-9P 345654-14-0P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)
RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Bhasin, C; Inorg chim Acta 1983, V77, PL31
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(9) Srivastava, S; Synth React inorg met-org Chem 1998, V28, P1431 HCAPLUS
(10) Srivastava, T; Indian J Chem 1983, V22A, P128 HCAPLUS
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(12) Srivastava, T; Indian J Chem 1983, V22A, P810 HCAPLUS

L8 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:583507 HCAPLUS
DN 115:183507
ED Entered STN: 01 Nov 1991
TI Reactions of (.eta.-methylcyclopentadienyl)manganese tricarbonyl with primary amines
AU **Srivastava, S. C.**; Shrimal, A. K.; Srivastava, Amar
CS Dep. Chem., Univ. Gorakhpur, Gorakhpur, India
SO Journal of Organometallic Chemistry (1991), 414(1), 65-9
CODEN: JORCAI; ISSN: 0022-328X
DT Journal
LA English
CC 29-11 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 23
OS CASREACT 115:183507
AB (.eta.-CH3C5H4)Mn(CO)3 reacts with RNH2 (R = n-C4H9, sec-C4H9, n-C5H11, n-C6H13, cyclo-C6H11, n-C7H15, n-C8H17, n-C9H19, C6H5CH2) to give corresponding sym-dialkylureas when a 1:2 M mixture of the two reactants is irradiated with UV light for 100-250 h. The complexes (.eta.-CH3C5H4)Mn(CO)2(CONHR)(H) were isolated for R = n-C4H9, n-C6H13, and cyclo-C5H11.
ST **urea** dialkyl; carbonylation amine manganese tricarbonyl
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. carbonylation of, by (methylcyclopentadienyl)manganese tricarbonyl, dialkylureas from)
IT Carbonylation
(photochem., of primary amines by (methylcyclopentadienyl)manganese tricarbonyl, dialkylureas from)
IT 12108-13-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(carbonylation by, of primary amines, photochem.)
IT 100-46-9, Benzylamine, reactions 108-91-8, Cyclohexylamine, reactions 109-73-9, Butylamine, reactions 110-58-7, Pentylamine 111-26-2, Hexylamine 111-68-2, Heptylamine 111-86-4, Octylamine 112-20-9, Nonylamine 13952-84-6, 2-Butanamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(carbonylation of, by (methylcyclopentadienyl)manganese tricarbonyl)
IT 869-79-4P 1466-67-7P 1792-17-2P 1798-20-5P 1943-08-4P 2078-76-4P 2387-23-7P 2763-88-4P 94381-33-6P 136638-43-2P 136638-44-3P 136638-45-4P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)

L8 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1984:195055 HCAPLUS
DN 100:195055
ED Entered STN: 08 Jun 1984
TI Preparation of molybdenum trisulfide by solid state chemical reactions
AU **Srivastava, S. K.**; Avasthi, B. N.; Basu, S.
CS Dep. Chem., Indian Inst. Technol., Kharagpur, 721302, India
SO Journal of Materials Science Letters (1984), 3(4), 313-14
CODEN: JMSLD5; ISSN: 0261-8028
DT Journal
LA English
CC 52-2 (Electrochemical, Radiational, and Thermal Energy Technology)
Section cross-reference(s): 49
AB Preparation of MoS3 (for battery cathodes and MoS2 manufacture) by the solid-state

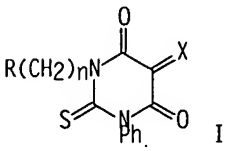
chemical reaction of MoO3 and **thiourea**, and characterization of the prepared MoS3 by chemical anal., x-ray study, thermogravimetric anal., magnetic susceptibility, IR spectra, etc. are reported.

ST molybdenum sulfide manuf battery cathode

IT Cathodes
(battery, molybdenum trisulfide for, preparation of)

IT 12033-29-3P
RL: **PREP (Preparation)**
(preparation of, by solid-state chemical reactions)

L8 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1984:156565 HCAPLUS
DN 100:156565
ED Entered STN: 12 May 1984
TI Substituted thiobarbituric acids as anti-Parkinsonian agents
AU Kumar, P.; **Nath, C.**; Agarwal, Jagdish C.; Bhargava, K. P.; Shanker, K.
CS Dep. Pharmacol. Ther., King George's Med. Coll., Lucknow, 226 003, India
SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1983), 22B(9), 955-8
CODEN: IJSBDB; ISSN: 0376-4699
DT Journal
LA English
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
OS CASREACT 100:156565
GI



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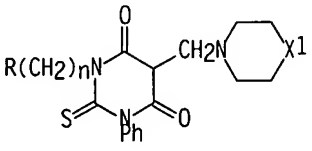

II

AB R(CH2)nNHCSNHPh (R = 2,4-Cl2C6H3, 3,5-Cl2C6H3, n = 0; R = 2,4-Cl2C6H3, 2,4-Me2C6H3, n = 1), prepared by the condensation of R(CH2)nNH2 with PhNCS, on cyclization with CH2(CO2H)2 in the presence of AcCl give the thiobarbituric acids I (X = H2), which are converted into I [X = CHR1, R1 = 4-MeOC6H4, 3,4-(MeO)2C6H3, 2-HOC6H4, 3-FC6H4, 3,4-MeO(HO)C6H3, 3,4-Cl2C6H3] and II (X1 = O,CH2, CH2CH2, NC6H4Cl-3) by Knoevenagel and Mannich reactions resp. Some of the compds. show significant anti-Parkinsonian activity with a high safety margin.

ST thiobarbiturate arylidene aminomethyl prepn Parkinsonism; arylidenethiobarbiturate prepn Parkinsonism; aminomethylthiobarbiturate prepn Parkinsonism

IT Parkinsonism
(inhibitor, arylidenethiobarbiturate and aminomethylthiobarbiturate)

IT 110-89-4, reactions 110-91-8, reactions 111-49-9 6640-24-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(aminomethylation of thiobarbiturate with)

IT 89516-52-9P 89516-53-0P 89516-54-1P 89516-55-2P 89516-56-3P
89516-57-4P 89516-58-5P 89516-59-6P 89516-60-9P 89516-61-0P
89516-62-1P 89516-63-2P 89516-64-3P 89516-65-4P 89516-66-5P
89516-67-6P 89516-68-7P 89516-69-8P 89516-70-1P 89516-71-2P

RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation and anti-Parkinsonism activity of)

IT 89516-48-3P 89516-49-4P 89516-50-7P 89516-51-8P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with aromatic aldehyde or formaldehyde and amine)

IT 13528-25-1P 62644-21-7P 89516-46-1P 89516-47-2P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with malonic acid)

IT 103-72-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aromatic amines)

IT 141-82-2, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with **arylthiourea**)

IT 94-98-4 95-00-1 554-00-7 626-43-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with pheny isothiocyanate)

IT 90-02-8, reactions 120-14-9 121-33-5 123-11-5, reactions 456-48-4 6287-38-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thiobarbiturate)

L8 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1976:150733 HCAPLUS
DN 84:150733
ED Entered STN: 12 May 1984
TI Reactions of aryl- and diarylthioureas with some molybdenum carbonyl derivatives
AU Tripathi, S. C.; **Srivastava, S. C.**; Pandey, R. D.; Mani, R. P.
CS Dep. Chem., Univ. Gorakhpur, Gorakhpur, India
SO Journal of Organometallic Chemistry (1976), 110(1), 67-71
CODEN: JORCAI; ISSN: 0022-328X
DT Journal
LA English
CC 29-11 (Organometallic and Organometalloidal Compounds)
AB Cycloheptatrienemolybdenum tricarbonyl reacted with ligands (L) (L = phenyl-, o-tolyl-, m-tolyl-, p-tolyl-, .alpha.-naphthyl-, .beta.-naphthyl-, sym-diphenyl-, sym-di-o-tolyl-, sym-di-p-tolyl- or sym-di-.alpha.-naphthyl-**thiourea**) to give Mo(CO)5L derivs. rather than the expected products, cis-Mo(CO)3L3. Evidence was obtained for the formation of trans-Mo(CO)4L2 derivs. when L = sym-diphenyl- and sym-di-o-tolyl-**thiourea**. These donors (L) on reaction with Mo(CO)4B(B = o-phenanthroline or 2,2'-bipyridine) yielded mixed ligand derivs. Mo(CO)3BL. The appearance of three C-O stretching bands in agreement with the Cs symmetry of mixed-ligand molybdenum carbonyls.
ST molybdenum **thiourea** carbonyl complex; phenanthroline **thiourea** molybdenum complex; bipyridine **thiourea** molybdenum complex
IT Carbonyls
RL: RCT (Reactant); RACT (Reactant or reagent)
(molybdenum, **thiourea** complexes)

IT 40419-06-5P 59244-68-7P 59244-69-8P 59244-70-1P 59244-71-2P
59244-72-3P 59244-73-4P 59244-74-5P 59244-75-6P 59244-76-7P
59244-77-8P 59244-78-9P 59244-79-0P 59244-80-3P 59244-81-4P
59244-82-5P 59244-83-6P 59527-11-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 15668-64-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with **phenylthiourea**)
IT 12125-77-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with **thiourea** derivs.)

L8 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1973:91955 HCAPLUS
DN 78:91955
ED Entered STN: 12 May 1984
TI Aryl- and diarylthioureamolybdenum carbonyls
AU Tripathi, S. C.; **Srivastava, S. C.**; Pandey, R. D.
CS Dep. Chem., Univ. Gorakhpur, Gorakhpur, India
SO Journal of Inorganic and Nuclear Chemistry (1973), 35(2), 457-63
CODEN: JINCAO; ISSN: 0022-1902
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 73
AB Ten aryl- and diarylthioureamolybdenum pentacarbonyls and 9 mixed derivs. [.pi.-C5H5Mo(CO)2L]2 (L = aryl or **diarylthiourea**) were synthesized. Bonding properties of these thioureas were interpreted by measurement of the ir spectra of synthesized substituted Mo carbonyls. The ir spectra of arylthioureamolybdenum pentacarbonyls had an addnl. C-O band in the low frequency side of the strongest peak. This addnl. C-O band was attributed to the lifting of the degeneracy of the E mode due to the unsym. structures of the arylthioureas. Two C-O bands observed in [.pi.-C5H5Mo(CO)2L]2 derivs. were attributed to modes (Au + Bu).
ST molybdenum **arylthiourea** carbonyl complex; **thiourea** aryl complex molybdenum; **urea** thio complex molybdenum; IR molybdenum **arylthiourea** carbonyl
IT Carbonyls
RL: RCT (Reactant); RACT (Reactant or reagent)
(molybdenum)
IT Force constant
Infrared spectra
(of molybdenum **arylthiourea** carbonyls)
IT 39385-34-7P 39385-35-8P 39385-36-9P 39385-45-0P 39385-46-1P
39385-47-2P 39385-48-3P 39385-50-7P 40419-02-1P 40419-03-2P
40419-04-3P 40419-05-4P 40419-06-5P 40419-07-6P 40419-08-7P
40419-09-8P 40419-10-1P 40530-62-9P 41482-09-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 12091-64-4 13939-06-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with arylthioureas)

L8 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1969:449887 HCAPLUS
DN 71:49887
ED Entered STN: 12 May 1984
TI Thiopegan derivatives. XXXV. Reaction between 6-aminopiperonal, and allyl isothiocyanate
AU Singh, Harjit; Singh, Ishwar; **Bhandari, K. S.**; Dhami, K. S.;

Arora, S. S.; Narang, K. S.
CS Panjab Univ., Chandigarh, India
SO Journal of the Indian Chemical Society (1969), 46(4), 367-70
CODEN: JICSAH; ISSN: 0019-4522
DT Journal
LA English
CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
AB Condensation of 6-aminopiperonal and allyl isothiocyanate furnished N-(2-formyl-4,5-methylenedioxyphenyl)-N-allyl **thiourea** which was cyclized to give 2-methyl-4-chloro-6,7-methylenedioxy-10,11-thiopega-9-ene hydrochloride and 2-bromomethyl-4-bromo-6,7-methylenedioxy-10,11-thiopega-9-ene by treatment with dry HCl gas and Br, resp. These products were condensed with some amines to introduce basic side chains at position 4.
ST thiazoloquinazolines; quinazolines thiazolo; thiopegan derivs
IT 23126-53-6P 23126-54-7P 23126-55-8P 23126-56-9P 23126-57-0P 23126-58-1P 23126-59-2P 23126-65-0P 23126-66-1P 23126-67-2P 23192-28-1P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
IT 57-06-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aminopiperonal)
IT 23126-68-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with isothiocyanic acid allyl ester)

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L13 ANSWER 1 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2004-213940 [20] WPIX
CR 2003-491702 [46]; 2003-851738 [79]
DNC C2004-084705
TI Preparation of pertinacious alkaline protease inhibitor useful as bio-control agent, involves the use of Streptomyces specie in fermentation medium containing assimilable carbon and nitrogen sources at specified conditions.
DC B04 C06 D16
IN DESHPANDE, V V; GHATGE, M S; RAO, M B; VERNEKAR, J V
PA (COUL) **COUNCIL SCI & IND RES CSIR**
CYC 1
PI US 2004038342 A1 20040226 (200420)* 5 C12N009-99
ADT US 2004038342 A1 Div ex US 2000-527602 20000317, US 2003-356576 20030203
FDT US 2004038342 A1 Div ex US 6514748
PRAI IN 1999-DE442 19990319
IC ICM C12N009-99
ICS C12N001-21
AB US2004038342 A UPAB: 20040324
NOVELTY - Preparing a pertinacious alkaline protease inhibitor comprising growing Streptomyces specie in a fermentation medium containing assimilable carbon and nitrogen sources at 28-30 deg. C for at least 96 hours, separating the solids by conventional methods to obtain a cell free liquid, and recovering a protease inhibitor by a precipitation method from the cell free liquid using salting out agent, is new.
ACTIVITY - Antifungal.
No biological data given.
MECHANISM OF ACTION - Pertinacious Alkaline Protease Inhibitor.
USE - The protrin inhibitor is useful as a bio-control agent or biodegradable antifungal agent (claimed).
ADVANTAGE - The invention provides an attractive and economical process for rapid and convenient production of protease inhibitor of microbial origin. It is easier to manipulate the microbial protease inhibitor than those from plants or animals sources. The alkaline protease inhibitor is biodegradable and environmentally friendly antifungal agent against toxic chemical fungicides used currently. It is stable over a pH of 6-12 and at 40-95 deg. C.
Dwg.0/0
FS CPI
FA AB; DCN
MC CPI: B04-A08C2; B04-A10; B04-C02B; B04-F10B5; B04-N02; B05-A01A; B05-A01B; B05-A03A; B05-B02A3; B05-C01; B05-C02; B05-C04; B05-C05; B05-C07; B07-A02A; B07-A02B; B10-A07; **B10-A13C**; B10-E04C; B11-B; B14-A04; B14-D07C; C04-A08C2; C04-A10; C04-C02B; C04-F10B5; C04-N02; C05-A01A; C05-A01B; C05-A03A; C05-B02A3; C05-C01; C05-C02; C05-C04; C05-C05; C05-C07; C07-A02A; C07-A02B; C10-A07; **C10-A13C**; C10-E04C; C11-B; C14-A04; C14-D07C; D05-C

L13 ANSWER 2 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2003-420291 [39] WPIX

DNC C2003-110706
TI Preparation of thiourea used for amino resin manufacture, involves passing carbon dioxide to mixture of carbon dioxide-hydrogen sulfide, adding calcium cyanamide, and passing carbon dioxide to decompose calcium compound.
DC E35
IN MORESHWAR, C G; MURTHY, B R K; PARSHURAM, K M; SHIVRAM, M S; SRINIVASA, B; YESHWANT, G M
PA (MORE-I) MORESHWAR C G; (MURT-I) MURTHY B R K; (PARS-I) PARSHURAM K M; (SHIV-I) SHIVRAM M S; (SRIN-I) SRINIVASA B; (YESH-I) YESHWANT G M; (COUL) **COUNCIL SCI & IND RES**
CYC 1
PI US 2003060662 A1 20030327 (200339)* 5 C07C335-00
US 6657082 B2 20031202 (200379) C07C335-02
ADT US 2003060662 A1 US 1998-46740 19980324; US 6657082 B2 US 1998-46740 19980324
PRAI US 1998-46740 19980324
IC ICM C07C335-00; C07C335-02
AB US2003060662 A UPAB: 20030619
NOVELTY - Improved process for the preparation of thiourea comprises passing a mixture of carbon dioxide and hydrogen sulfide into a slurry formed by addition of calcium cyanamide into water, separating the thiourea solution, treating with activated carbon, removing the carbon, separating the product and drying the product at a temperature between 50 to 70 deg. C to obtain the product.

DETAILED DESCRIPTION - An improved process for the preparation of thiourea which comprises passing a mixture of carbon dioxide and hydrogen sulfide into a slurry formed by addition of calcium cyanamide into water under constant stirring, maintaining alkaline pH at a temperature ranging between ambient to 80 deg. C, stopping the addition of hydrogen sulfide, continuing the slow passing of carbon dioxide and addition of remaining part of calcium cyanamide charge and retaining reaction mass to complete the secondary reactions to form the product for a period ranging from 2 to 5 hours and continuing passing of carbon dioxide at an increased rate for effecting decomposition of Ca(SH)2 for a period of 1.6 to 6 hours, stopping the addition of carbon dioxide, separating the thiourea solution, treating the separated solution with activated carbon, removing the carbon, separating the product formed and drying the product at a temperature between 50 to 70 deg. C to obtain the product.

USE - For preparing thiourea used for manufacturing amino resins, herbicides, fungicides, insecticides, plant growth regulators and photographic papers, and for electrochemical processes, pharmaceutical industries, textile processing, hydrometallurgy, rubber industry and petroleum industry.

ADVANTAGE - High purity thiourea is produced in a high yield, by the improved process.

Dwg.0/0
FS CPI
FA AB; DCN
MC CPI: **E10-A13A1**; E11-F09

L13 ANSWER 3 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2003-267864 [26] WPIX
DNN N2003-213028 DNC C2003-069743
TI Process for isolation of p-benzosemiquinone, for measuring toxicity of cigarette, involves collecting tar or cigarette smoke solution, extracting using methylene chloride, water saturated n-butanol and purifying.

DC D18 E14 J04 P15 S03
IN CHATTERJEE, I B
PA (COUL) **COUNCIL SCI & IND RES**
CYC 101
PI WO 2003000633 A2 20030103 (200326)* EN 83 C07C037-00
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TR TZ UG ZM ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT RO RU SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG US UZ VN YU ZA ZM ZW
US 2003111087 A1 20030619 (200341) A24F001-00
EP 1402253 A2 20040331 (200424) EN G01N031-00
R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT RO SE SI TR
KR 2004019316 A 20040305 (200444) C07C037-00
US 6782891 B2 20040831 (200457) G01N033-497
AU 2002232115 A1 20030108 (200460) C07C037-00
US 2004204617 A1 20041014 (200468) C07C037-68
ADT WO 2003000633 A2 WO 2002-IN19 20020131; US 2003111087 A1 US 2002-76033 20020213; EP 1402253 A2 EP 2002-712239 20020131, WO 2002-IN19 20020131; KR 2004019316 A KR 2003-716754 20031222; US 6782891 B2 US 2002-76033 20020213; AU 2002232115 A1 AU 2002-232115 20020131; US 2004204617 A1 Div ex US 2002-76033 20020213, US 2004-754025 20040108
FDT EP 1402253 A2 Based on WO 2003000633; AU 2002232115 A1 Based on WO 2003000633
PRAI IN 2001-DE701 20010622
IC ICM A24F001-00; C07C037-00; C07C037-68; G01N031-00; G01N033-497
ICS A24F001-10
AB WO2003000633 A UPAB: 20031030
NOVELTY - Process for isolation of p-benzosemiquinone involves collecting tar or cigarette smoke solution, extracting with potassium phosphate buffer, methylene chloride and water saturated n-butanol, subjecting to thin layer chromatography using silica plates which are developed, identifying location of band corresponding to Rf 0.26, extracting with acetone and water saturated n-butanol, and drying.

DETAILED DESCRIPTION - A tar or cigarette smoke solution is collected from lighted conventional filtered tipped cigarettes. The tar is collected by lighting the cigarettes having a tar content of 20-30 mg/cigarette in a glass flask dipped in a mixture of ice and salt. The tar is allowed to condense and settle at the bottom of the flask. The flask is kept at room temperature and the tar is extracted using 30-60 mM potassium phosphate buffer at a pH of 7.4-7.8.

The resulting solution is filtered through 0.45 micro m Millipore filter and the pH of the filtrate is adjusted to 7.4-7.6 by adding sodium hydroxide solution. The tar solution is extracted thrice with equal volume of methylene chloride. The lower methylene chloride layer is discarded and the upper yellow colored aqueous layer termed as aqueous extract of cigarette smoke is collected. The aqueous extract is extracted twice with equal volume of water saturated n-butanol. The cooled yellow butanol extract is lyophilized in a lyophilizer at -50 deg. C to -60 deg. C under vacuum.

The lyophilized material is extracted twice with high performance liquid chromatography (HPLC) grade acetone. The acetone solution is dried under vacuum, and the acetone extract is dissolved with HPLC grade methanol. The methanol solution is subjected to band thin layer

chromatography using non-fluorescent silica plates.

The plates are developed using a mixture of toluene and ethylacetate in a ratio of 80:20. The plate is taken out and dried at 25-30 deg. C using a drier. Small strips containing the developed material is cut from both sides of the plates, and are kept in an iodine chamber for the location of band corresponding to Rf 0.26. The band is scrapped and extracted with HPLC grade acetone. The acetone layer is collected and dried under vacuum. The acetone extract which appeared as pale yellow needles is dissolved by adding equal volume of milli Q water.

The resultant aqueous solution is extracted with equal volume of HPLC grade water saturated n-butanol. The upper n-butanol layer is dried in small glass tubes under vacuum to obtain the major cigarette smoke (cs) oxidant with a purity of 98-99% and yield of 18-22 micro g/cigarette. The (cs) oxidant is purified by dissolving a mobile solvent comprising a mixture of methylene chloride and methanol in a volume ratio of 90:50.

The resulting solution is injected in a HPLC instrument with a normal phase 20 cm silica column using an ultraviolet detector at 294 nm at a flow rate of 0.5 ml/minute, and at 25 deg. C and 29 kgf/cm2. The effluent which appears as a single peak at a retention time of 8.80 minute is collected with a purity of 100% and yield of 8.4% of the total cs oxidant present in parent tar solution. The (cs) oxidant is p-benzosemiquinone which is responsible for the oxidative damage of proteins and deoxynucleic acid (DNA).

INDEPENDENT CLAIMS are also included for:

(1) a process for quantitative determination of p-benzosemiquinone;

(2) a method for prevention of cigarette smoke induced protein oxidation in vitro;

(3) use of chemical compounds or agents selected from ascorbic acid, sodium dithionite, tartaric acid, citric acid, oxalic acid, succinic acid, histidine, lysine, thiourea, glutathione, black tea extract, green tea extract, catechin, epigallocatechin and epicatechin, as antidote for the harmful effect caused by the cigarette smoke oxidant;

(4) use of p-benzosemiquinone compound; and

(5) method for quantitative estimation of p-benzosemiquinone.

USE - For isolating p-benzosemiquinone for studying mechanism of oxidative damage-induced degenerative diseases caused by cigarette smoke reducing oxidative damage to isolated protein, DNA, culture cell or to an experimental model under laboratory conditions, and for formulating the quantity and nature of smoking material to be used in cigarette, cigar, cigarette pipes and other conventional smoking devices.

ADVANTAGE - p-Benzosemiquinone which is a harmful oxidant from cigarette is isolated with high purity and high yield.

DESCRIPTION OF DRAWING(S) - The figure shows the high performance liquid chromatography of the butanol extract after thin layer chromatography.

Dwg.3/35

FS CPI EPI GMPI

FA AB; GI; DCN

MC CPI: D07-C; D07-D; E06-A01; E07-A02B; E07-D09B; E10-A01; **E10-A13A2** ; E10-B01C1; E10-C02D1; E10-C02D2; E10-C02F; E10-E04L3; E10-F02C; E10-H04C4; E11-Q01; E11-Q03C; E31-F04; E31-K05D; J04-B01C

EPI: S03-E09C3; S03-E09C5; S03-E13D; S03-E14A

L13 ANSWER 4 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN

AN 2002-163234 [21] WPIX

DNC C2002-050358

TI New composition for a slow release nitrogenous fertilizer e.g. urea

comprises an inert material and an essential oil or its derivatives.
DC C04
IN AGARWAL, K K; ANWAR, M; KHANUJA, S P S; KIRAN, U; KUMAR, S; PATRA, D D; SINGH, A
PA (COUL) **COUNCIL SCI & IND RES**
CYC 1
PI US 6336949 B1 20020108 (200221)* 7 C05C009-00
ADT US 6336949 B1 US 1999-263791 19990305
PRAI IN 1999-DE324 19990212
IC ICM C05C009-00
ICS C05G005-00
AB US 6336949 B UPAB: 20031030
NOVELTY - A slow release nitrogenous fertilizer composition comprises a nitrogenous fertilizer, an inert material (0.5 - 1 w/w%) and an essential oil or its derivatives (0.5 - 1 w/w%).
DETAILED DESCRIPTION - An INDEPENDENT CLAIM is included for preparing the composition involving:
(a) coating the nitrogenous fertilizer with an inert material;
(b) air drying the coated fertilizer for 24 hours;
(c) further coating the coated fertilizer of step (b) with the essential oil or its derivatives; and
(d) air drying the coated fertilizer of step (c) for 24 hours.
ACTIVITY - None given.
MECHANISM OF ACTION - Urease and nitrification inhibitor.
USE - For slow release of nitrogenous fertilizer e.g. urea (claimed).
ADVANTAGE - The composition acts as a cheap and eco-friendly urease/nitrification inhibitor. The components are easily decomposable, thus do not leave adverse influence in soil. The composition is as effective as dicyanodiamide as nitrification inhibitor and does not allow higher accumulation of NH4-N following hydrolysis of urea.
Dwg.0/0
FS CPI
FA AB; DCN
MC CPI: C04-B01C1; **C10-A13C**; C12-M10A; C14-T04

L13 ANSWER 5 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2002-129541 [17] WPIX
DNC C2002-039641
TI A fertilizer comprising an ammonium-producing fertilizer, benzotriazole and chelating agent in a specific ratio as a nitrification inhibiting additive is new.
DC C04
IN GOWDA, N M N; KUMAR, S; PUTTAN, K; RAO, E V S P
PA (COUL) **COUNCIL SCI & IND RES**
CYC 1
PI US 6331198 B1 20011218 (200217)* 4 C05B007-00
ADT US 6331198 B1 US 1999-273361 19990322
PRAI IN 1999-DE232 19990212
IC ICM C05B007-00
ICS C05C009-00
AB US 6331198 B UPAB: 20031030
NOVELTY - A fertilizer comprises an ammonium-producing fertilizer and a nitrification-inhibiting additive. The additive comprises (weight%) benzotriazole (a) (2.5 - 50) and chelating agent (b) (1 - 50).
ACTIVITY - Fertilizer.
MECHANISM OF ACTION - Nitrification inhibitor.
USE - As nitrification inhibiting additive for ammonium-producing

fertilizers (claimed).
ADVANTAGE - The combination of (a) and (b) provides the synergistic activity of the additive. Better inhibition of nitrification is achieved which reduces nitrogen losses and economizes nitrogen use. Benzotriazole is used in lower concentrations and shows an increased efficiency when combined with metal ion chelating compounds. The nitrification inhibitor amends nitrogen fertilizers to improve crop yields, increases fertilizer use efficiency, reduces nitrate content in food and improves quality of agriculture produce. The combination of benzotriazole and the chelating agent is a superior nitrification inhibiting additive for ammonium-producing fertilizer than either benzotriazole or chelating agent used separately.
Dwg.0/0

FS CPI
FA AB; DCN
MC CPI: C06-D08; C10-A03; **C10-A13A**; **C10-A13C**; C10-A18; C10-A20; C10-B01B; C14-L06; C14-T03

L13 ANSWER 6 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2001-626239 [72] WPIX
DNC C2001-186536
TI Fertilizer, useful as a nitrification and urease inhibitor, comprises a nitrogenous fertilizer, castor oil and oil derived from Artemisia annua.
DC C04
IN ANWAR, M; CHAND, S; KIRAN, U; KUMAR, S; PATRA, D D
PA (COUL) **COUNCIL SCI & IND RES**; (COUL) **COUNCIL SCI & IND RES INDIANA**
CYC 90
PI WO 2001072665 A1 20011004 (200172)* EN 22 C05G003-08
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW NL OA PT SD SE SL SZ TZ UG ZW
W: AE AL AM AT AU AZ BA BB BG BR BY CA CH CN CR CU CZ DE DK DM EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZW
AU 2000054250 A 20011008 (200208) C05G003-08
US 6315807 B1 20011113 (200225)# C05G003-00
BR 2000006931 A 20020423 (200235) C05G003-08
CN 1354736 A 20020619 (200263) C05G003-08
CA 2338454 C 20041214 (200501) EN C05C009-00
ADT WO 2001072665 A1 WO 2000-IN32 20000328; AU 2000054250 A AU 2000-54250 20000328, WO 2000-IN32 20000328; US 6315807 B1 US 2000-536752 20000328; BR 2000006931 A BR 2000-6931 20000328, WO 2000-IN32 20000328; CN 1354736 A CN 2000-801156 20000328, WO 2000-IN32 20000328; CA 2338454 C CA 2000-2338454 20000328, WO 2000-IN32 20000328
FDT AU 2000054250 A Based on WO 2001072665; BR 2000006931 A Based on WO 2001072665; CA 2338454 C Based on WO 2001072665
PRAI WO 2000-IN32 20000328; US 2000-536752 20000328
IC ICM C05C009-00; C05G003-00; C05G003-08
ICS C05C003-00
AB WO 200172665 A UPAB: 20011206
NOVELTY - A novel fertilizer useful as a nitrification and urease inhibitor is new.
DETAILED DESCRIPTION - A novel fertilizer useful as a nitrification and urease inhibitor comprises a nitrogenous fertilizer, castor oil and oil derived from Artemisia annua. INDEPENDENT CLAIMS are included for:
(i) a method for producing the fertilizer comprising application of

castor oil and Artemisia annua oil to a nitrogenous fertilizer; and
(ii) a method of using Artemisia oil as a urease and nitrification inhibitor comprising coating urea or other ammonium forming fertilizer granules with 1% castor oil and 0.5 to 5% Artemisia oil.
USE - The fertilizer is useful as a nitrification and urease inhibitor.
ADVANTAGE - The product is as effective as dicyandiamide as a nitrification inhibitor, has higher urease inhibitory activity, is natural and low persistence, doesn't allow high accumulation and consequent loss of ammonia and is cheaper than many synthetic inhibitors.
Dwg.0/0
FS CPI
FA AB; DCN
MC CPI: C04-B01C1; C05-C01; **C10-A13C**; C14-D07; C14-T01; C14-T03; C14-T04

L13 ANSWER 7 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 1997-312699 [29] WPIX
DNC C1997-100764
TI Process to prepare polymers of low molecular weight - comprises polymerisation of the monomer in the presence of an electron donor, an electron acceptor and a free radical quencher.
DC A18 A97 E19 H07
IN PANDURANGARAO, S; SURIANARAYANAN, M; VIJARAGHAVAN, K; VIJAYARAGHAVAN, R; RAO, S P; VIJAYARAGHAVAN, K
PA (COUL) **COUNCIL SCI & IND RES**; (COUL) **CSIR COUNCIL SCI IND RES**
CYC 4
PI EP 779299 A1 19970618 (199729)* EN 7 C08F002-06
R: DE FR GB
US 5998555 A 19991207 (200004)# C08F002-06
EP 779299 B1 20010704 (200138) EN C08F002-06
R: DE FR GB
DE 69521619 E 20010809 (200153) C08F002-06
ADT EP 779299 A1 EP 1995-308998 19951211; US 5998555 A US 1995-560403 19951117; EP 779299 B1 EP 1995-308998 19951211; DE 69521619 E DE 1995-621619 19951211, EP 1995-308998 19951211
FDT DE 69521619 E Based on EP 779299
PRAI EP 1995-308998 19951211; US 1995-560403 19951117
REP 1.Jnl.Ref; FR 1561315
IC ICM C08F002-06
ICS C08K005-08
AB EP 779299 A UPAB: 20031105
A process for the preparation of a polymer comprises carrying out, in solution, polymerisation of the desired monomer or monomers in the presence of a complex of an electron donor and an electron acceptor which complex is capable of dissociating to release a free radical and a cation and a free radical quencher.
USE - The polymers of low molecular weight are used as additives in the petroleum industry, as pour point depressants, viscosity improvers or antioxidants.
ADVANTAGE - The process enhances polymer yield and gives a polymer having a low polydispersity index and low molecular weight.
Dwg.0/0
FS CPI
FA AB; DCN
MC CPI: A02-A03; A10-B01; A10-D; E07-D13B; E10-A06A; **E10-A13B2**;

E10-A19B; E10-B04D; E10-E02D5; E10-E02F1; E10-H04C1; E10-H04C4; E10-H04D2; H07-G01; H07-G05; H07-G06

L13 ANSWER 8 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 1991-185259 [25] WPIX
CR 1992-079509 [10]; 1994-248456 [30]
DNC C1991-080221
TI Cyclohexyl EDTA mono anhydride - which forms radio metal chelates capable of surviving in vivo.
DC B03 B04 K08
IN MEASE, R C; **SRIVASTAVA, S C**
PA (UYAS-N) ASSOC UNIV INC
CYC 1
PI US 5021571 A 19910604 (199125)*
ADT US 5021571 A US 1989-372905 19890629
PRAI US 1989-372905 19890629
IC C07D265-30
AB US 5021571 A UPAB: 19940921
Cyclohexyl EDTA monoanhydride is claimed.
ADVANTAGE - These ligands will form radiometal chelates that are capable of surviving in-vivo, by combining the rigidity of the ligand with the general utility of polyaminocarboxylates. These semi-rigid chelates can bind the radiometal, can be conjugated to monoclonal antibodies, and overcome the stability problems of prior art materials. Many of the complexes are more stable in serum than those formed using non-rigid chelates such as EDTA and DTPA.
In an example, mixture of trans-1,2-diaminocyclohexane -N,N,N',N'-tetraacetic acid (4.3g), pyridine (4.0 ml) and acetic anhydride (9.4 ml) was stirred at room temperature for 24 hrs.. The slurry was filtered and washed extensively with acetic acid and then diethyl ether. The off white solid was collected and dried under vacuum to give trans-1,2-diamino cyclohexane-N,N,N',N'-tetraacetic acid monoanhydride (CDTAMA, 1.7g, 41%, m.pt. 235-238 deg C). Concentration of the filtrate yielded an organe sticky solid which was washed with cold methylene chloride to give the dianhydride (1.2g, 31%, m.pt. 179-183 deg.C as an off white solid, CDTAMA in DMSO was added to the anticolon CA17-1A antibody (20 mg/ml in 0.1N sodium bicarbonate) at a molar ratio of CDTAMA/antibody of 10/1. The solution was allowed to incubate at 4 deg C overnight. @(9pp Dwg.No.0/0)
0/0
FS CPI
FA AB; DCN
MC CPI: B05-A04; B07-D03; B07-E03; B10-A04; B10-A12C; **B10-A13A**; B10-A14; B10-A19; B10-B01B; B12-K04A1; K09-B; K09-E

L13 ANSWER 9 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 1986-107222 [17] WPIX
DNC C1986-045823
TI Separating mixture of alpha-olefin(s) and N-paraffin(s) from coker distillate - or other complex cracked prod. mixed by adduction with large excess of urea and decomposition with e.g. water.
DC E17 H04
IN BHATTACHAR, K K; JOSHI, G C; KULSRESTHA, G N; SAXENA, M P
PA (COUL) **COUNCIL OF SCIENTIFIC & IND RES**
CYC 1
PI DE 3436289 A 19860417 (198617)* 24
PRAI DE 1984-3436289 19841003
IC C07C007-15; C07C009-14; C07C011-02; C07C015-02; C10G053-08; C10G067-06

AB DE 3436289 A UPAB: 19990127
Selective separation of linear terminal olefin mixts. plus n-paraffins from petroleum distillate fractions comprises: (i) adding to cracked 6-20C distillates 4-8 pts. urea per pt. additive-forming hydrocarbons in presence of excess of activators and organic solvents; (ii) separating the adducts formed; and (iii) breaking down the adducts conventionally.

The activator (added at a concentration of 30-250 volume/weight%) may include methanol, ethanol, propanol, methyl ethyl ketone, methyl isobutyl ketone or water. The solvent may be ethylene glycol, furfural, phenol, hydrocarbons (e.g. pentane, benzene, toluene, light naphtha), chlorinated hydrocarbons (e.g. CH2Cl2) or non-adducted raffinate.

USE/ADVANTAGE - The process can be applied to naphtha, kerosene and gas oil and the like obtd. by cracking and especially coking of crude oil fractions. The olefins obtd. are useful in production of oxo alcohols, detergents, synthetic lubricants, additives, etc. The urea adduction technique is here applied for the first time to this type of feedstock, containing complex mixts. of cpds. The prod. after removal of soluble impurities, contains less than 3 weight% branched mols., less than 2 weight% diolefins and less than 1.0 weight% aromatics.

Dwg.0/0

FS CPI
FA AB
MC CPI: **E10-A13B**; E10-J02C3; E10-J02D; H02-D02

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=> d his

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L1           58 E3-8
                E SRIVASTAVA S/AU
L2         2243 E3-22
                E SRIVASTAVA SHIPRA/AU
L3            1 E3
                E NATH C/AU
L4           67 E3-4
L5         8868 (COUNC? (1A) SCI? (1A) IND? (1A) RES?)/CS,PA
L6           32 L1-4 AND ?UREA/BI
L7            0 L6 AND ?ARYLOXY?/BI
L8           11 L6 AND PREP+NT/RL

     FILE 'WPIX' ENTERED AT 12:29:11 ON 03 FEB 2005
                E BHANDARI K/AU
                E SRIVASTAVA S/AU
L9           91 E3-10
                E NATH C/AU
L10           4 E3
L11        1163 (COUNC? (1A) SCI? (1A) IND? (1A) RES?)/CS,PA
L12       25583 (B10-A13? OR C10-A13? OR E10-A13?)/MC OR (C07C273 OR C07C275)/I
L13           9 L9-11 AND L12

     FILE 'REGISTRY' ENTERED AT 12:37:10 ON 03 FEB 2005

     FILE 'HCAPLUS' ENTERED AT 12:37:15 ON 03 FEB 2005
L14             TRA L8 1- RN :      245 TERMS

     FILE 'REGISTRY' ENTERED AT 12:37:16 ON 03 FEB 2005
L15          245 SEA L14
L16              STR
L17            0 L16
L18           26 L16 FULL
                SEL RN 3-18 22
L19           17 E1-17 AND L18

     FILE 'HCAPLUS' ENTERED AT 13:13:51 ON 03 FEB 2005
L20            2 L19
L21            0 L20 AND L1-5

     FILE 'HCAOLD' ENTERED AT 13:14:39 ON 03 FEB 2005
L22            0 L19

=> b reg
FILE 'REGISTRY' ENTERED AT 13:16:08 ON 03 FEB 2005
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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STRUCTURE FILE UPDATES: 1 FEB 2005 HIGHEST RN 824390-04-7
DICTIONARY FILE UPDATES: 1 FEB 2005 HIGHEST RN 824390-04-7

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Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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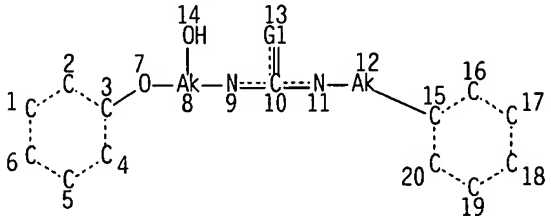
L16 STR



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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 15 3
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
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L19 17 SEA FILE=REGISTRY ABB=ON PLU=ON (245483-91-4/BI OR 335022-01-0/BI OR 335022-03-2/BI OR 335022-07-6/BI OR 335022-09-8/BI OR 335022-11-2/BI OR 335022-13-4/BI OR 335022-15-6/BI OR 335022-19-0/BI OR 335022-25-8/BI OR 335022-27-0/BI OR 335022-31-6/BI OR 335022-33-8/BI OR 335022-35-0/BI OR 335022-37-2/BI OR 335022-39-4/BI OR 335022-43-0/BI) AND L18

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FILE COVERS 1907 - 3 Feb 2005 VOL 142 ISS 6
FILE LAST UPDATED: 2 Feb 2005 (20050202/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L20 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:97882 HCAPLUS
DN 134:316232
ED Entered STN: 09 Feb 2001
TI Liquid chromatographic enantioseparation of .beta.-blocking agents with (1R,2R)-1,3-diacetoxy-1-(4-nitrophenyl)-2-propyl isothiocyanate as chiral derivatizing agent
AU Peter, M.; Gyeresi, A.; Fulop, F.
CS Institute of Pharmaceutical Chemistry, University of Szeged, Szeged, H-6720, Hung.
SO Journal of Chromatography, A (2001), 910(2), 247-253
CODEN: JCRAEY; ISSN: 0021-9673
PB Elsevier Science B.V.
DT Journal
LA English
CC 64-3 (Pharmaceutical Analysis)
AB The applicability of (1R,2R)-1,3-diacetoxy-1-(4-nitrophenyl)-2-Pr isothiocyanate [(R,R)-DANI] as a recently developed chiral derivatizing agent for the enantiosepn. of a series of .beta.-blockers is described. The thiourea diastereomers formed were analyzed by reversed-phase high-performance liquid chromatog., mixts. of water and methanol or acetonitrile being used for elution. Conditions of derivatization (temperature, reagent excess and reaction time) were optimized, and the effects of organic modifiers on the retention and separation were investigated; the diastereomers could readily be baseline separated with methanol-containing mobile phases with resolns. between 1.58 and 2.72.
ST beta blocker resoln HPLC chiral agent; isothiocyanate chiral agent sepn adrenoceptor antagonist
IT Reversed phase HPLC
(enantiosepn. of .beta.-blockers by reversed phase HPLC using (R,R)-DANI as chiral derivatizing agent)
IT Adrenoceptor antagonists
(.beta.-; enantiosepn. of .beta.-blockers by reversed phase HPLC using (R,R)-DANI as chiral derivatizing agent)
IT 525-66-6 3930-20-9 6452-71-7 13523-86-9 13655-52-2 29122-68-7
36894-69-6 37517-30-9 51384-51-1 63659-18-7 66515-26-2
335021-83-5 335021-99-3 **335022-01-0** **335022-03-2**
335022-05-4 **335022-07-6** **335022-09-8**
335022-11-2 **335022-13-4** **335022-15-6**
335022-17-8 **335022-19-0** 335022-21-4 335022-23-6
335022-25-8 **335022-27-0** 335022-29-2
335022-31-6 **335022-33-8** **335022-35-0**
335022-37-2 **335022-39-4** 335022-41-8

335022-43-0 335022-45-2 335022-48-5 335022-50-9
RL: ANT (Analyte); ANST (Analytical study)
(enantiosepn. of .beta.-blockers by reversed phase HPLC using
(R,R)-DANI as chiral derivatizing agent)
IT 250265-34-0
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(enantiosepn. of .beta.-blockers by reversed phase HPLC using
(R,R)-DANI as chiral derivatizing agent)
RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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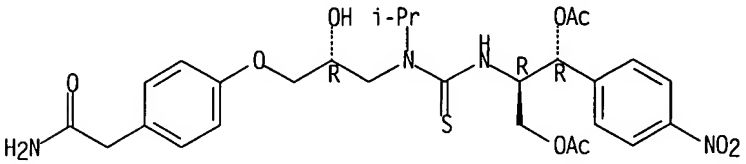
IT 335022-01-0 335022-03-2 335022-07-6
335022-09-8 335022-11-2 335022-13-4
335022-15-6 335022-19-0 335022-25-8
335022-27-0 335022-31-6 335022-33-8
335022-35-0 335022-37-2 335022-39-4
335022-43-0
RL: ANT (Analyte); ANST (Analytical study)

(enantiosepn. of .beta.-blockers by reversed phase HPLC using (R,R)-DANI as chiral derivatizing agent)

RN 335022-01-0 HCAPLUS

CN Benzeneacetamide, 4-[(2R)-3-[[[[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]amino]thioxomethyl](1-methylethyl)amino]-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)

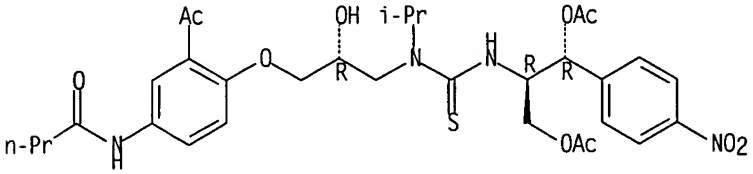
Absolute stereochemistry.



RN 335022-03-2 HCAPLUS

CN Butanamide, N-[3-acetyl-4-[(2R)-3-[[[[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]amino]thioxomethyl](1-methylethyl)amino]-2-hydroxypropoxy]phenyl]- (9CI) (CA INDEX NAME)

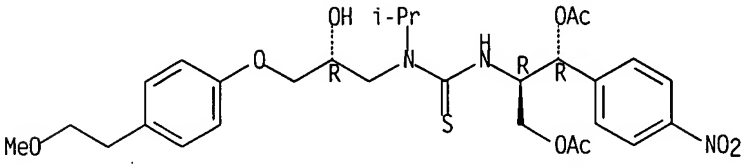
Absolute stereochemistry.



RN 335022-07-6 HCAPLUS

CN Thiourea, N'-[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]-N-[(2R)-2-hydroxy-3-[4-(2-methoxyethyl)phenoxy]propyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

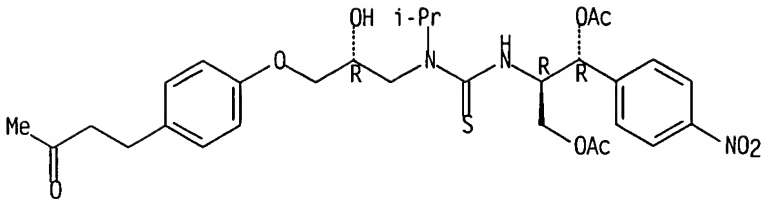
Absolute stereochemistry.



RN 335022-09-8 HCAPLUS

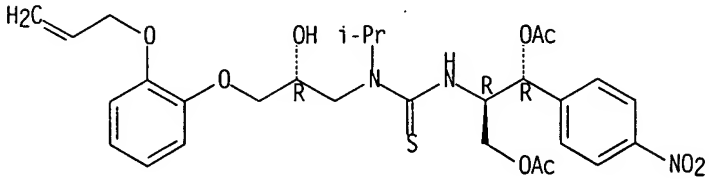
CN Thiourea, N'-[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]-N-[(2R)-2-hydroxy-3-[4-(3-oxobutyl)phenoxy]propyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 335022-11-2 HCAPLUS
CN Thiourea, N'-[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]-N-[(2R)-2-hydroxy-3-[2-(2-propenyloxy)phenoxy]propyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

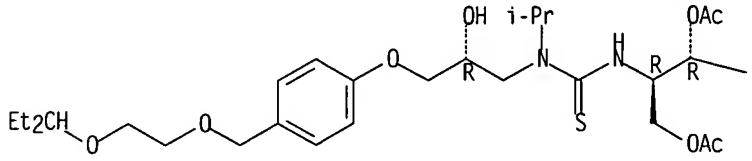
Absolute stereochemistry.



RN 335022-13-4 HCAPLUS
CN Thiourea, N'-[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]-N-[(2R)-3-[4-[[2-(1-ethylpropoxy)ethoxy]methyl]phenoxy]-2-hydroxypropyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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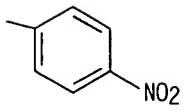
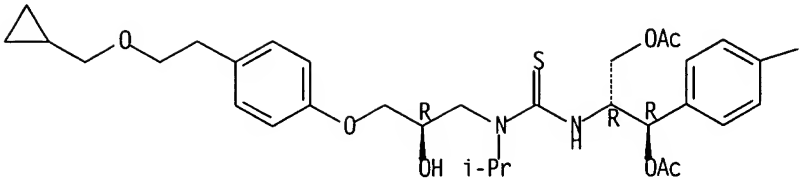


RN 335022-15-6 HCAPLUS
CN Thiourea, N'-[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]-N-[(2R)-3-[4-[2-(cyclopropylmethoxy)ethyl]phenoxy]-2-hydroxypropyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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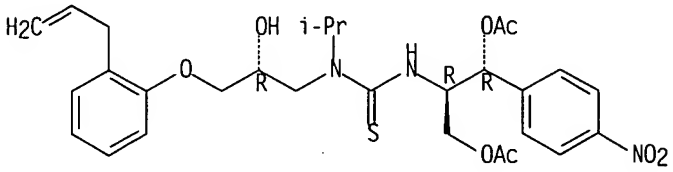
—NO_2

RN 335022-19-0 HCAPLUS
CN Thiourea, N'-[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]-N-[(2R)-2-hydroxy-3-[2-(2-propenyl)phenoxy]propyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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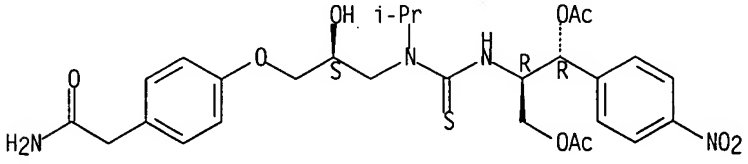
CN Benzeneacetamide, 4-[(2S)-3-[[[[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]amino]thioxomethyl](1-methylethyl)amino]-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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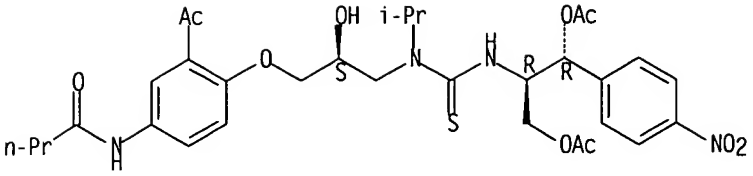
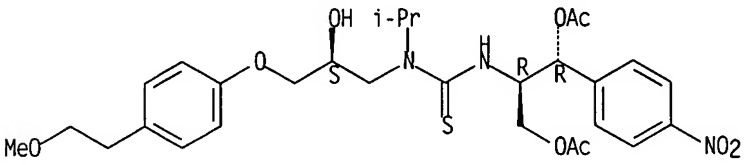
CN Butanamide, N-[3-acetyl-4-[(2S)-3-[[[[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]amino]thioxomethyl](1-methylethyl)amino]-2-hydroxypropoxy]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



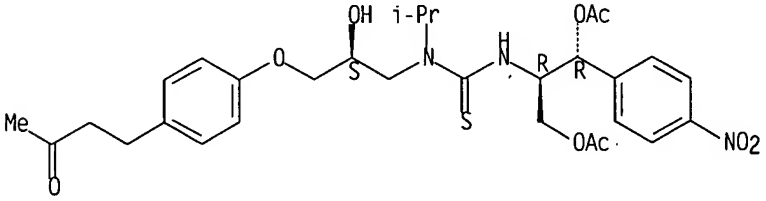
RN 335022-31-6 HCAPLUS
CN Thiourea, N'-[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]-N-[(2S)-2-hydroxy-3-[4-(2-methoxyethyl)phenoxy]propyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 335022-33-8 HCAPLUS
CN Thiourea, N'-[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]-N-[(2S)-2-hydroxy-3-[4-(3-oxobutyl)phenoxy]propyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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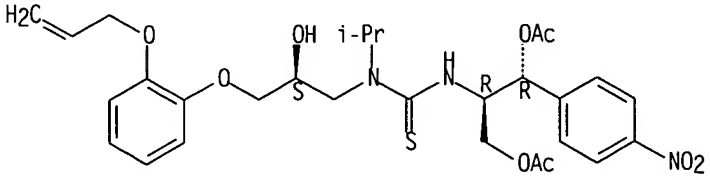
CN Thiourea, N'-[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]-N-[(2S)-2-hydroxy-3-[2-(2-propenyloxy)phenoxy]propyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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CN Thiourea, N'-[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]-N-[(2S)-3-[4-[[2-(1-ethylpropoxy)ethoxy]methyl]phenoxy]-

2-hydroxypropyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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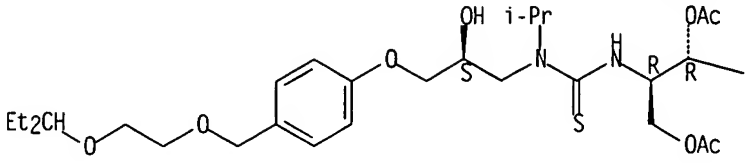
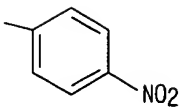


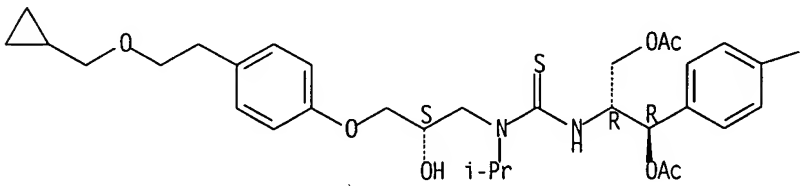
PAGE 1-B



RN 335022-39-4 HCAPLUS
CN Thiourea, N'-[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]-N-[(2S)-3-[4-[2-(cyclopropylmethoxy)ethyl]phenoxy]-2-hydroxypropyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

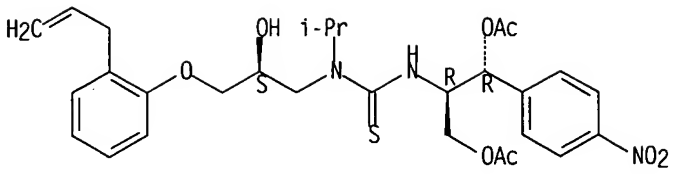
PAGE 1-A



PAGE 1-B

RN 335022-43-0 HCAPLUS
CN Thiourea, N'-[(1R,2R)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-(4-nitrophenyl)ethyl]-N-[(2S)-2-hydroxy-3-[2-(2-propenyl)phenoxy]propyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L20 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:640828 HCAPLUS
DN 131:272178
ED Entered STN: 08 Oct 1999
TI Preparation of N-(mercaptoalkyl)urea derivatives of amino acids as inhibitors of TNF-.alpha. production
IN Mita, Shiro; Horiuchi, Masato; Ban, Masakazu; Suhara, Hiroshi
PA Santen Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 324 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC ICM C07C323-44
ICS C07C327-22; C07C329-06; C07C275-16; C07C275-24; C07D213-40; C07D233-61; C07D295-12; C07D295-18; C07F007-18; A61K031-17; A61K031-415; A61K031-44; A61K031-445; A61K031-495; A61K031-595
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1
FAN.CNT 1

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PI	WO 9950238	A1	19991007	WO 1999-JP1554	19990325
	W: CA, CN, KR, NO, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	JP 2000044533	A2	20000215	JP 1999-78346	19990323
	JP 3603177	B2	20041222		
	CA 2325741	AA	19991007	CA 1999-2325741	19990325
	EP 1072591	A1	20010131	EP 1999-910724	19990325
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	US 6492370	B1	20021210	US 2000-623779	20000908
	US 2002198376	A1	20021226	US 2002-147131	20020515
	US 6730784	B2	20040504		
PRAI	JP 1998-79154	A	19980326		
	WO 1999-JP1554	W	19990325		
	US 2000-623779	A3	20000908		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9950238	ICM	C07C323-44
	ICS	C07C327-22; C07C329-06; C07C275-16; C07C275-24; C07D213-40; C07D233-61; C07D295-12; C07D295-18; C07F007-18; A61K031-17; A61K031-415; A61K031-44; A61K031-445; A61K031-495; A61K031-595
WO 9950238	ECLA	C07C317/50; C07C329/06; C07D295/18B1F; C07D333/32; C07C323/44; C07C323/59; C07C327/30

EP 1072591	ECLA	C07C317/50; C07C323/44; C07C323/59; C07C323/60; C07C327/30; C07C329/06; C07D295/18B1F; C07D033/32
US 6492370	ECLA	C07C317/50; C07C323/44; C07C323/59; C07C323/60; C07C327/30; C07C329/06; C07D295/18B1F; C07D033/32
US 2002198376	ECLA	C07C317/50; C07C323/44; C07C323/59; C07C323/60; C07C327/30; C07C329/06; C07D295/18B1F; C07D033/32

OS MARPAT 131:272178

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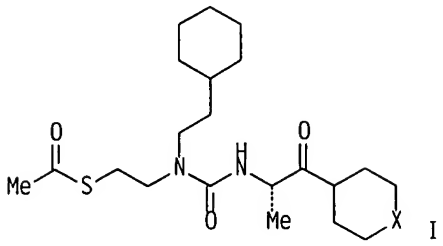

I

AB Prepared are .alpha.-[N'-(mercaptoalkyl)ureido]alkanamide compds. having a urea structure as the basic structure and carrying sulfur and amide bonds in side chains. The above compds. are represented by general formula R1S-A1(R7)-NR2CONR3-A2(R4)CONR5R6 [wherein R1 represents H, (un)substituted lower alkyl or aromatic group, RA-CO-, RC-S- or a group of formula S-A1(R7)-NR2CONR3-A2(R4)CONR5R6; R2, R3 and R4 represent each H, (un)substituted lower alkyl or alkenyl, cycloalkyl, cycloalkenyl or (un)substituted aromatic group; R5 and R6 represent each H, (un)substituted lower alkyl or alkenyl, cycloalkyl, cycloalkenyl or (un)substituted aromatic group, or R5 and R6 may form together (un)substituted nonarom. heterocycle; R7 represents H, (un)substituted lower alkyl, cycloalkyl, hydroxy, mercapto, Ph, RB-O-, RC-S-, RD-COS-, RE-OCO-, RF-N(RG)- or -CONHOH; A1 and A2 represent each an alkylene; RA represents lower (halo)alkyl, aromatic group, lower alkoxy, aromatic-lower alkoxy, RF, or NRG; RB represents lower alkyl or aromatic group; RC represents H, lower alkyl, aromatic group; RD represents lower alkyl or aromatic group; RE represents H, lower alkyl, or aromatic group, RF and RG represent H, lower alkyl, cycloalkyl, or aromatic group]. It has been found out that these compds. have pharmacol. effects, in particular, a tumor necrosis factor-.alpha. (TNF-.alpha.) production inhibitory effect. They are useful as remedies for autoimmune diseases and as antirheumatics. Thus, (2S)-2-[3-[2-(acetylthio)ethyl]-3-(2-cyclohexylethyl)ureido]propionic acid (preparation given) was condensed with N-methylpiperazine using 1-hydroxybenzotriazole, 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride, and N-methylmorpholine in CH2Cl2 at room temperature overnight to give the title compound (I; X = NMe) in 78% yield. I (X = NMe) and I (X = O) at 50 mg/kg p.o. inhibited the Salmonella lipopolysaccharide-induced production of TNF-.alpha. in rats by 84.6 and 93.5%, resp.

ST mercaptoalkylurea amino acid deriv prepn antirheumatic; autoimmune disease treatment mercaptoalkylureidoalkanamide; TNF prodn inhibitor mercaptoalkylureidoalkanamide

IT Antirheumatic agents
Autoimmune disease
(preparation of N-(mercaptoalkyl)urea derivs. of amino acids as inhibitors of TNF-.alpha. production, antirheumatics, and remedies for autoimmune disease)

IT Tumor necrosis factors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of N-(mercaptoalkyl)urea derivs. of amino acids as inhibitors of TNF-.alpha. production, antirheumatics, and remedies for autoimmune disease)

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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-(mercaptoalkyl)urea derivs. of amino acids as inhibitors of TNF-.alpha. production, antirheumatics, and remedies for autoimmune

disease)

IT 96-33-3, Methyl acrylate 98-88-4, Benzoyl chloride 100-51-6, Benzyl alcohol, reactions 100-53-8, Benzyl mercaptan 100-60-7, N-Methylcyclohexylamine 103-63-9, Phenethyl bromide 107-85-7, Isopentylamine 108-00-9, 2-(Dimethylamino)ethylamine 108-18-9, Diisopropylamine 108-24-7, Acetic anhydride 108-95-2, Phenol, reactions 109-01-3, N-Methylpiperazine 109-73-9, n-Butylamine, reactions 109-85-3, 2-Methoxyethylamine 124-40-3, reactions 124-63-0, Methanesulfonyl chloride 141-43-5, 2-Aminoethanol, reactions 501-53-1, Benzyloxycarbonyl chloride 504-78-9, Thiazolidine 507-09-5, Thioacetic acid, reactions 530-62-1, 1,1'-Carbonyl diimidazole 590-86-3, Isovaleraldehyde 593-51-1, Methylamine hydrochloride 949-99-5 1138-80-3, N-(Benzyloxycarbonyl)glycine 1647-26-3, 2-Cyclohexylethyl bromide 2346-00-1, 2-Methylthiazoline 5470-11-1, Hydroxylamine hydrochloride 10593-85-8 13404-22-3 13518-40-6 24424-99-5, Di-tert-butyl dicarbonate 33305-77-0 39684-80-5, N-(tert-Butoxycarbonyl)-(2-bromoethyl)amine 53990-33-3 73311-57-6 75646-21-8 86864-60-0 100564-78-1 142003-32-5 174626-26-7 245489-26-3 245489-36-5 245489-44-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of N-(mercaptoalkyl)urea derivs. of amino acids as inhibitors of TNF-.alpha. production, antirheumatics, and remedies for autoimmune disease)

IT 122-98-5P 1738-78-9P, L-Phenylalanine benzyl ester p-toluenesulfonate 3529-10-0P, 4-(Dimethylamino)butylamine 3911-27-1P 6404-30-4P 6950-53-4P 10578-75-3P, [2-(Benzyloxy)ethyl]amine hydrochloride 15028-41-8P, Methyl 2-amino-2-methylpropanoate hydrochloride 15911-75-8P 16874-17-2P 17083-22-6P 22572-33-4P, [2-(Benzylthio)ethyl]amine hydrochloride 28607-46-7P, D-Phenylalanine benzyl ester p-toluenesulfonate 30250-67-0P 34946-13-9P 37089-43-3P 37880-99-2P 42854-62-6P, L-Alanine benzyl ester p-toluenesulfonate 53934-77-3P 53934-78-4P 58576-72-0P 60116-06-5P 61275-22-7P 61487-52-3P 65096-31-3P 73995-16-1P 75190-94-2P 85262-29-9P 93564-26-2P 94912-71-7P 104217-35-8P 110755-67-4P 110755-68-5P 125483-58-1P 137381-03-4P 138374-03-5P 139397-46-9P 141630-12-8P, L-Phenylalanine phenyl ester hydrochloride 147864-79-7P 162083-21-8P 186431-76-5P 186489-67-8P 208468-67-1P 219496-44-3P 245480-15-3P 245480-16-4P 245480-17-5P 245480-18-6P 245480-19-7P 245480-20-0P 245480-21-1P 245480-22-2P 245480-23-3P 245480-24-4P 245480-25-5P 245480-26-6P 245480-27-7P 245480-28-8P 245480-29-9P 245480-30-2P 245480-31-3P 245480-32-4P 245480-33-5P 245480-34-6P 245480-35-7P 245480-36-8P 245480-37-9P 245480-38-0P 245480-39-1P 245480-40-4P 245480-41-5P 245480-42-6P 245480-43-7P 245480-44-8P 245480-45-9P 245480-46-0P 245480-47-1P 245480-48-2P 245480-49-3P 245480-50-6P 245480-51-7P 245480-52-8P 245480-53-9P 245480-54-0P 245480-55-1P 245480-56-2P 245480-57-3P 245480-59-5P 245480-60-8P 245480-61-9P 245480-62-0P 245480-63-1P 245480-65-3P 245480-66-4P 245480-67-5P 245480-68-6P 245480-70-0P 245480-71-1P 245480-72-2P 245480-73-3P 245480-74-4P 245480-75-5P 245480-76-6P 245480-77-7P 245480-78-8P 245480-79-9P 245480-80-2P 245480-81-3P 245480-82-4P 245480-83-5P 245480-84-6P 245480-85-7P 245480-86-8P 245480-87-9P 245480-88-0P 245480-89-1P 245480-90-4P 245480-91-5P 245480-92-6P 245480-94-8P 245480-95-9P 245480-96-0P 245480-97-1P 245480-98-2P 245480-99-3P 245481-00-9P 245481-01-0P 245481-02-1P 245481-03-2P 245481-04-3P 245481-05-4P 245481-07-6P 245481-08-7P 245481-09-8P 245481-10-1P 245481-11-2P 245481-12-3P 245481-13-4P 245481-14-5P 245481-15-6P 245481-16-7P 245481-17-8P 245481-18-9P 245481-19-0P 245481-20-3P 245481-21-4P

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245482-91-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-(mercaptoalkyl)urea derivs. of amino acids as inhibitors of TNF-.alpha. production, antirheumatics, and remedies for autoimmune disease)

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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-(mercaptoalkyl)urea derivs. of amino acids as inhibitors of TNF-.alpha. production, antirheumatics, and remedies for autoimmune disease)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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(2) American Cyanamid Co; US 5312831 A HCAPLUS
(3) American Cyanamid Co; EP 652228 A1 HCAPLUS
(4) American Cyanamid Co; AU 669064 B HCAPLUS
(5) American Cyanamid Co; HU 67038 T HCAPLUS
(6) American Cyanamid Co; FI 9402186 A HCAPLUS
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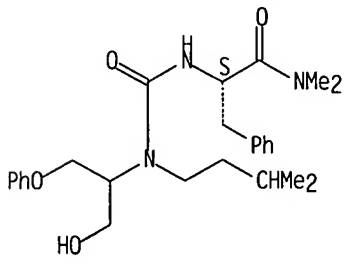
(14) Japan Tobacco Inc; WO 9708133 A1 HCAPLUS
(15) Japan Tobacco Inc; JP 09118658 A 1997 HCAPLUS

IT **245483-91-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-(mercaptoalkyl)urea derivs. of amino acids as inhibitors of TNF-.alpha. production, antirheumatics, and remedies for autoimmune disease)

RN 245483-91-4 HCAPLUS

CN Benzenepropanamide, .alpha.-[[[[1-(hydroxymethyl)-2-phenoxyethyl](3-methylbutyl)amino]carbonyl]amino]-N,N-dimethyl-, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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